Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Diisopropyl-3,6-dimethoxynaphthalene-2,7-disulfonamide

Zu-Wei Song[a] and Zhi-Qiang Hu[b]*

[a]College of Science, Qingdao Agricultural University, Qingdao 266109, People's Republic of China, and [b]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China
Correspondence e-mail: songzuwei2008@yahoo.cn

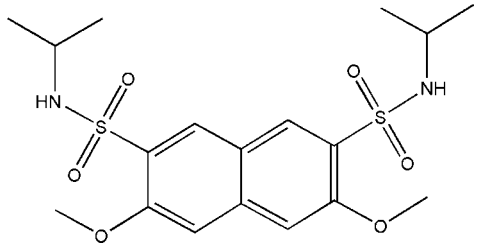
Received 6 July 2008; accepted 8 July 2008

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.117; data-to-parameter ratio = 19.3.

In the title compound, $C_{18}H_{26}N_2O_6S_2$, all bond lengths and angles are normal. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds.

Related literature

For the crystal structures of related compounds, see: Henschel *et al.* (1996). For details of the biological activities of fluorine-containing compounds, see: Kamoshita *et al.* (1987). For catalytic activity, see: Zhang *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{26}N_2O_6S_2$
M_r = 430.53
Monoclinic, $P2_1/c$
a = 17.229 (3) Å
b = 7.2532 (15) Å
c = 18.035 (4) Å
β = 108.35 (3)°
V = 2139.2 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 173 (2) K
0.50 × 0.38 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.871, T_{max} = 0.940
8740 measured reflections
4889 independent reflections
4227 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.117
S = 1.16
4889 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.88	2.00	2.821 (2)	154
N2—H2B···O5^{ii}	0.88	2.22	3.001 (2)	148
N2—H2B···O6^{ii}	0.88	2.53	3.235 (2)	138

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, -y+2, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2423).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Henschel, D., Hiemisch, O., Blaschette, A. & Jones, P. G. (1996). *Z. Naturforsch. Teil B*, **51**, 1313–1315.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Kamoshita, K., Matsumoto, H. & Nagano, E. (1987). US Patent No. 4 670 046.
Rigaku (2004). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, Z. B., Zhou, S. Y. & Nie, J. (2007). *J. Mol. Catal. A Chem.* **265**, 9–14.

supporting information

Acta Cryst. (2008). E**64**, o1499 [doi:10.1107/S1600536808021211]

N,*N*′-Diisopropyl-3,6-dimethoxynaphthalene-2,7-disulfonamide

Zu-Wei Song and Zhi-Qiang Hu

S1. Comment

The sulfonamides form an important group in organic chemistry with many compounds containing sulfonamide groups possessing a broad spectrum of biological activities and can be widely used as herbicides (Kamoshita *et al.*, 1987). In addition, some compounds containing sulfonimide groups can be used as catalysts (Zhang *et al.*, 2007). Here, we report the crystal structure of the title compound, (I).

In (I) (Fig. 1), all bond lengths are normal (Allen *et al.*, 1987) and in good agreement with those reported previously (Henschel *et al.*, 1996). As can be seen from the packing diagram (Fig. 2), the crystal structure of (I) is stabilized by intermolecular N—H···O hydrogen bonding. The crystal packing is further stabilized by van der Waals forces

S2. Experimental

A solution of naphthalene disulfonyl chloride (384 mg, 1 mmol) dissolved in anhydrous CH_2Cl_2 (10 ml), and dropwise added over a period of 10 min to a solution of propan-2-amine (118 mg, 2 mmol) in CH_2Cl_2 (10 ml) at 273 K. The mixture was stirred at r.t. for 4 h. The organic phase was washed with water twice, and dried over anhydrous Na_2SO_4. The solvent was removed and the residue was purified by flash chromatography (1:3 cyclohexane:dichloromethane) to give) as a white solid (267 mg, 62%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol and dichloromethane at room temperature.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95–1.0 Å and N—H = 0.88 Å with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C,*N*).

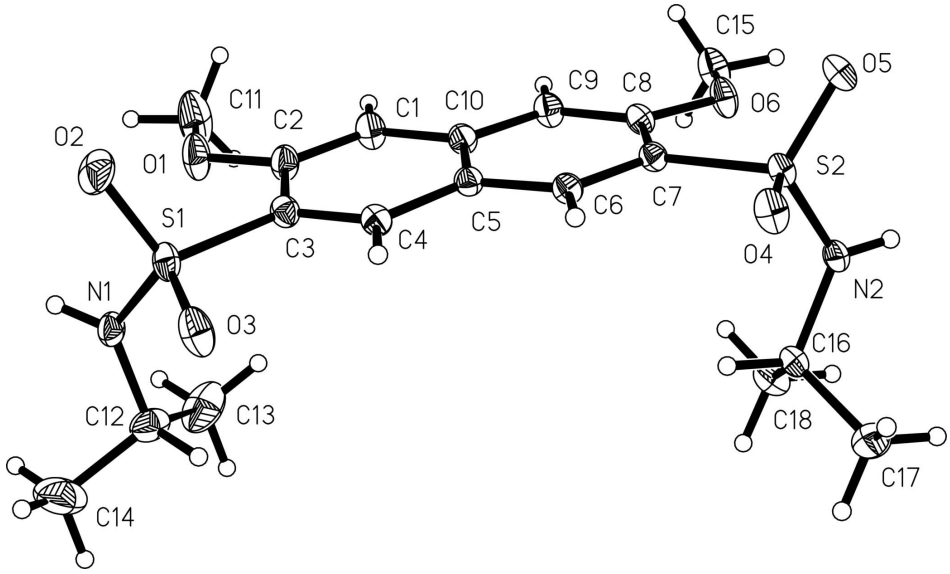


Figure 1

The molecular structure of (I), with atom labels and 40% probability displacement ellipsoids for non-H atoms.

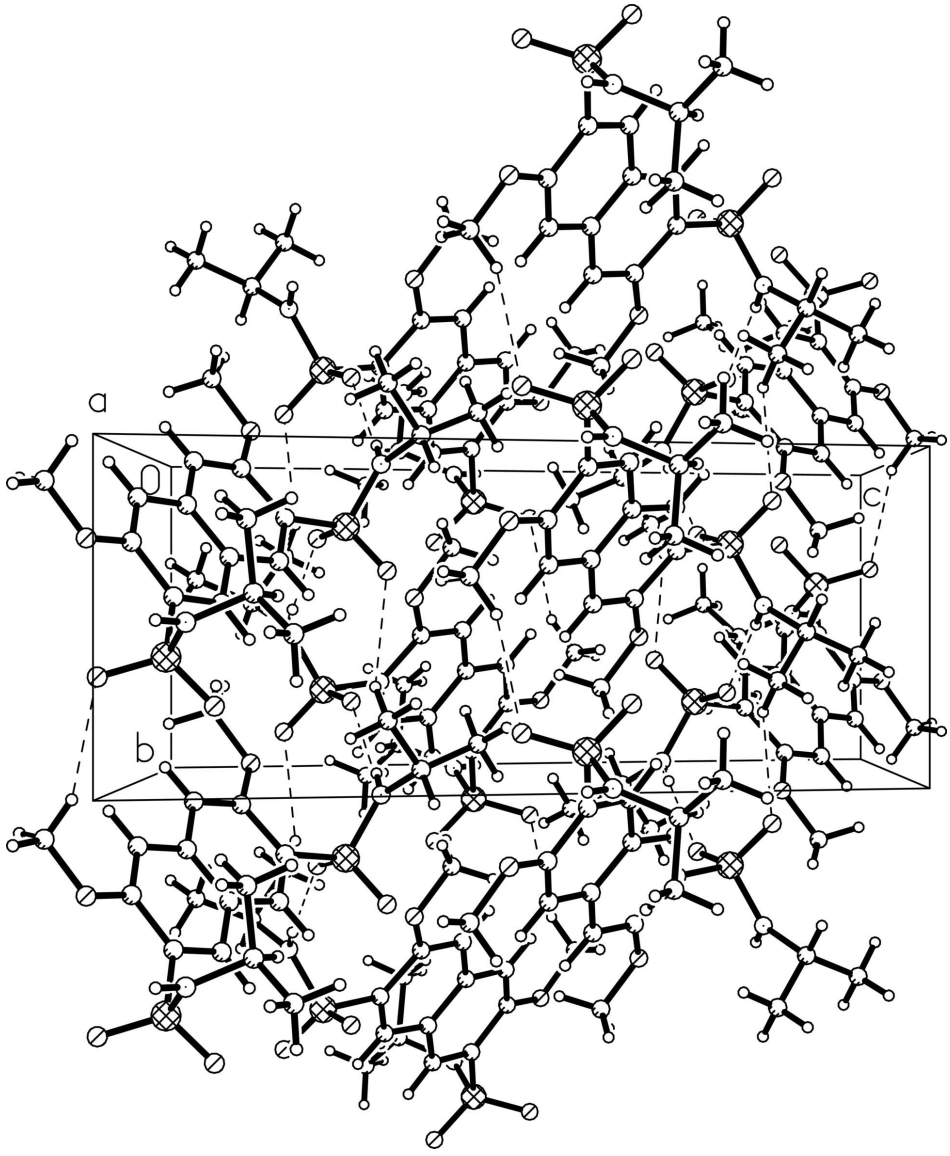


Figure 2

The packing of (I), viewed down the *a* axis, showing one layer of molecules connected by N—H···O hydrogen bonds (dashed lines).

N,*N*′-Diisopropyl-3,6-dimethoxynaphthalene-2,7-disulfonamide

Crystal data

$C_{18}H_{26}N_2O_6S_2$
M_r = 430.53
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 17.229 (3) Å
b = 7.2532 (15) Å
c = 18.035 (4) Å
β = 108.35 (3)°
V = 2139.2 (8) Å^3
Z = 4
$F(000)$ = 912
D_x = 1.337 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 875 reflections
θ = 2.2–27.5°
μ = 0.28 mm^{-1}
T = 173 K
Plate, colorless
0.50 × 0.38 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Radiation source: rotating anode
Graphite monochromator
ω scans at fixed $\chi = 45°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.871$, $T_{max} = 0.940$

8740 measured reflections
4889 independent reflections
4227 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.3°$
$h = -22 \rightarrow 22$
$k = -9 \rightarrow 9$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.117$
$S = 1.16$
4889 reflections
253 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.9298P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.39879 (3)	0.72730 (7)	0.23076 (3)	0.02292 (13)
S2	0.08210 (3)	1.11117 (7)	0.42543 (3)	0.01969 (13)
O1	0.42832 (10)	0.4396 (2)	0.35142 (10)	0.0368 (4)
O2	0.48381 (9)	0.7597 (2)	0.27099 (10)	0.0365 (4)
O3	0.35149 (10)	0.8610 (2)	0.17682 (9)	0.0325 (4)
O4	0.08620 (9)	1.2491 (2)	0.36997 (9)	0.0277 (3)
O5	0.09471 (9)	1.1659 (2)	0.50512 (8)	0.0261 (3)
O6	0.12159 (9)	0.7784 (2)	0.52066 (8)	0.0268 (3)
N1	0.39535 (10)	0.5367 (2)	0.18585 (10)	0.0232 (4)
H1A	0.4415	0.4763	0.1933	0.028*
N2	−0.00546 (10)	1.0136 (2)	0.39554 (9)	0.0223 (4)
H2B	−0.0358	1.0076	0.4266	0.027*
C1	0.33009 (13)	0.5414 (3)	0.41377 (13)	0.0280 (5)
H1B	0.3424	0.4413	0.4496	0.034*
C2	0.37011 (13)	0.5567 (3)	0.35894 (13)	0.0262 (4)
C3	0.35006 (12)	0.7046 (3)	0.30358 (11)	0.0212 (4)

C4	0.29442 (12)	0.8349 (3)	0.30760 (11)	0.0209 (4)
H4B	0.2823	0.9338	0.2712	0.025*
C5	0.25444 (11)	0.8252 (3)	0.36502 (11)	0.0197 (4)
C6	0.19712 (11)	0.9599 (3)	0.37008 (11)	0.0197 (4)
H6A	0.1874	1.0640	0.3365	0.024*
C7	0.15537 (11)	0.9418 (3)	0.42305 (11)	0.0190 (4)
C8	0.16906 (12)	0.7855 (3)	0.47337 (11)	0.0215 (4)
C9	0.22660 (13)	0.6566 (3)	0.47142 (12)	0.0247 (4)
H9A	0.2370	0.5553	0.5066	0.030*
C10	0.27065 (12)	0.6734 (3)	0.41739 (11)	0.0222 (4)
C11	0.4475 (2)	0.2809 (4)	0.40126 (18)	0.0543 (8)
H11A	0.4905	0.2093	0.3897	0.081*
H11B	0.3985	0.2044	0.3922	0.081*
H11C	0.4666	0.3207	0.4560	0.081*
C12	0.32048 (14)	0.4553 (3)	0.13290 (14)	0.0336 (5)
H12A	0.2781	0.5540	0.1156	0.040*
C13	0.28821 (17)	0.3054 (4)	0.1736 (2)	0.0527 (8)
H13A	0.2766	0.3573	0.2191	0.079*
H13B	0.3292	0.2075	0.1905	0.079*
H13C	0.2379	0.2541	0.1374	0.079*
C14	0.3397 (2)	0.3816 (5)	0.06177 (16)	0.0605 (9)
H14A	0.3603	0.4820	0.0368	0.091*
H14B	0.2899	0.3305	0.0246	0.091*
H14C	0.3813	0.2847	0.0780	0.091*
C15	0.12852 (15)	0.6187 (3)	0.56924 (14)	0.0333 (5)
H15A	0.0910	0.6304	0.6001	0.050*
H15B	0.1848	0.6082	0.6044	0.050*
H15C	0.1145	0.5083	0.5364	0.050*
C16	−0.03619 (12)	0.9332 (3)	0.31603 (11)	0.0237 (4)
H16A	0.0085	0.9406	0.2917	0.028*
C17	−0.10837 (15)	1.0449 (4)	0.26648 (13)	0.0365 (6)
H17A	−0.0915	1.1732	0.2642	0.055*
H17B	−0.1527	1.0400	0.2897	0.055*
H17C	−0.1276	0.9935	0.2135	0.055*
C18	−0.05611 (15)	0.7314 (3)	0.32295 (13)	0.0315 (5)
H18A	−0.0071	0.6671	0.3553	0.047*
H18B	−0.0746	0.6756	0.2708	0.047*
H18C	−0.0995	0.7212	0.3472	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0250 (3)	0.0202 (3)	0.0293 (3)	−0.00251 (19)	0.0167 (2)	−0.0004 (2)
S2	0.0251 (3)	0.0173 (2)	0.0197 (2)	0.00184 (18)	0.01134 (18)	−0.00043 (19)
O1	0.0400 (9)	0.0387 (10)	0.0408 (9)	0.0213 (8)	0.0256 (8)	0.0147 (8)
O2	0.0269 (8)	0.0371 (10)	0.0497 (10)	−0.0128 (7)	0.0179 (7)	−0.0073 (8)
O3	0.0468 (10)	0.0232 (8)	0.0372 (9)	0.0067 (7)	0.0270 (8)	0.0073 (7)
O4	0.0373 (8)	0.0209 (8)	0.0307 (8)	0.0051 (6)	0.0192 (7)	0.0061 (6)

O5	0.0350 (8)	0.0238 (8)	0.0229 (7)	−0.0010 (6)	0.0143 (6)	−0.0054 (6)
O6	0.0377 (9)	0.0218 (8)	0.0297 (8)	0.0051 (6)	0.0232 (7)	0.0056 (6)
N1	0.0204 (8)	0.0233 (9)	0.0278 (9)	0.0050 (7)	0.0100 (7)	−0.0020 (7)
N2	0.0211 (8)	0.0296 (10)	0.0197 (8)	0.0004 (7)	0.0114 (7)	−0.0028 (7)
C1	0.0325 (12)	0.0280 (12)	0.0270 (10)	0.0091 (9)	0.0144 (9)	0.0078 (9)
C2	0.0250 (10)	0.0278 (11)	0.0284 (10)	0.0074 (8)	0.0120 (8)	0.0032 (9)
C3	0.0222 (10)	0.0210 (10)	0.0223 (9)	−0.0023 (8)	0.0099 (8)	−0.0008 (8)
C4	0.0227 (10)	0.0199 (10)	0.0210 (9)	−0.0019 (8)	0.0084 (8)	−0.0012 (8)
C5	0.0197 (9)	0.0207 (10)	0.0191 (9)	−0.0006 (7)	0.0069 (7)	−0.0003 (8)
C6	0.0218 (10)	0.0195 (10)	0.0187 (9)	−0.0003 (7)	0.0076 (7)	0.0015 (8)
C7	0.0208 (9)	0.0173 (9)	0.0193 (9)	0.0009 (7)	0.0070 (7)	−0.0012 (7)
C8	0.0256 (10)	0.0227 (10)	0.0189 (9)	−0.0004 (8)	0.0108 (8)	−0.0001 (8)
C9	0.0302 (11)	0.0229 (11)	0.0239 (10)	0.0047 (8)	0.0126 (9)	0.0048 (8)
C10	0.0233 (10)	0.0232 (10)	0.0211 (9)	0.0012 (8)	0.0085 (8)	−0.0003 (8)
C11	0.0676 (19)	0.0501 (17)	0.0593 (17)	0.0394 (15)	0.0400 (15)	0.0280 (14)
C12	0.0292 (12)	0.0283 (12)	0.0356 (12)	0.0092 (9)	−0.0008 (9)	−0.0077 (10)
C13	0.0341 (14)	0.0359 (15)	0.085 (2)	−0.0089 (11)	0.0150 (14)	−0.0131 (15)
C14	0.066 (2)	0.068 (2)	0.0356 (14)	0.0236 (17)	0.0000 (14)	−0.0182 (15)
C15	0.0495 (14)	0.0233 (11)	0.0372 (12)	0.0038 (10)	0.0281 (11)	0.0065 (10)
C16	0.0251 (10)	0.0297 (11)	0.0182 (9)	0.0022 (8)	0.0097 (8)	−0.0024 (8)
C17	0.0359 (13)	0.0399 (14)	0.0288 (11)	0.0101 (10)	0.0031 (10)	0.0007 (10)
C18	0.0407 (13)	0.0282 (12)	0.0264 (11)	−0.0013 (10)	0.0119 (10)	−0.0041 (9)

Geometric parameters (Å, º)

S1—O3	1.4324 (16)	C8—C9	1.371 (3)
S1—O2	1.4345 (17)	C9—C10	1.416 (3)
S1—N1	1.5937 (18)	C9—H9A	0.9500
S1—C3	1.775 (2)	C11—H11A	0.9800
S2—O4	1.4320 (15)	C11—H11B	0.9800
S2—O5	1.4402 (15)	C11—H11C	0.9800
S2—N2	1.5984 (18)	C12—C13	1.512 (4)
S2—C7	1.772 (2)	C12—C14	1.520 (4)
O1—C2	1.353 (2)	C12—H12A	1.0000
O1—C11	1.434 (3)	C13—H13A	0.9800
O6—C8	1.356 (2)	C13—H13B	0.9800
O6—C15	1.434 (3)	C13—H13C	0.9800
N1—C12	1.466 (3)	C14—H14A	0.9800
N1—H1A	0.8800	C14—H14B	0.9800
N2—C16	1.483 (2)	C14—H14C	0.9800
N2—H2B	0.8800	C15—H15A	0.9800
C1—C2	1.377 (3)	C15—H15B	0.9800
C1—C10	1.418 (3)	C15—H15C	0.9800
C1—H1B	0.9500	C16—C17	1.517 (3)
C2—C3	1.432 (3)	C16—C18	1.517 (3)
C3—C4	1.364 (3)	C16—H16A	1.0000
C4—C5	1.415 (3)	C17—H17A	0.9800
C4—H4B	0.9500	C17—H17B	0.9800

C5—C6	1.412 (3)	C17—H17C	0.9800
C5—C10	1.420 (3)	C18—H18A	0.9800
C6—C7	1.371 (3)	C18—H18B	0.9800
C6—H6A	0.9500	C18—H18C	0.9800
C7—C8	1.424 (3)		

O3—S1—O2	120.31 (10)	C1—C10—C5	119.10 (18)
O3—S1—N1	108.65 (10)	O1—C11—H11A	109.5
O2—S1—N1	105.52 (10)	O1—C11—H11B	109.5
O3—S1—C3	105.36 (9)	H11A—C11—H11B	109.5
O2—S1—C3	106.66 (10)	O1—C11—H11C	109.5
N1—S1—C3	110.17 (9)	H11A—C11—H11C	109.5
O4—S2—O5	118.63 (9)	H11B—C11—H11C	109.5
O4—S2—N2	108.82 (10)	N1—C12—C13	110.9 (2)
O5—S2—N2	106.76 (9)	N1—C12—C14	108.1 (2)
O4—S2—C7	105.99 (9)	C13—C12—C14	111.5 (2)
O5—S2—C7	109.31 (9)	N1—C12—H12A	108.8
N2—S2—C7	106.79 (9)	C13—C12—H12A	108.8
C2—O1—C11	118.22 (18)	C14—C12—H12A	108.8
C8—O6—C15	117.67 (16)	C12—C13—H13A	109.5
C12—N1—S1	124.38 (14)	C12—C13—H13B	109.5
C12—N1—H1A	117.8	H13A—C13—H13B	109.5
S1—N1—H1A	117.8	C12—C13—H13C	109.5
C16—N2—S2	120.79 (13)	H13A—C13—H13C	109.5
C16—N2—H2B	119.6	H13B—C13—H13C	109.5
S2—N2—H2B	119.6	C12—C14—H14A	109.5
C2—C1—C10	120.7 (2)	C12—C14—H14B	109.5
C2—C1—H1B	119.6	H14A—C14—H14B	109.5
C10—C1—H1B	119.6	C12—C14—H14C	109.5
O1—C2—C1	125.2 (2)	H14A—C14—H14C	109.5
O1—C2—C3	115.08 (18)	H14B—C14—H14C	109.5
C1—C2—C3	119.73 (19)	O6—C15—H15A	109.5
C4—C3—C2	120.08 (18)	O6—C15—H15B	109.5
C4—C3—S1	118.62 (15)	H15A—C15—H15B	109.5
C2—C3—S1	121.27 (15)	O6—C15—H15C	109.5
C3—C4—C5	121.11 (19)	H15A—C15—H15C	109.5
C3—C4—H4B	119.4	H15B—C15—H15C	109.5
C5—C4—H4B	119.4	N2—C16—C17	109.64 (17)
C6—C5—C4	121.62 (18)	N2—C16—C18	108.73 (17)
C6—C5—C10	119.25 (17)	C17—C16—C18	113.51 (19)
C4—C5—C10	119.10 (18)	N2—C16—H16A	108.3
C7—C6—C5	120.63 (18)	C17—C16—H16A	108.3
C7—C6—H6A	119.7	C18—C16—H16A	108.3
C5—C6—H6A	119.7	C16—C17—H17A	109.5
C6—C7—C8	120.15 (18)	C16—C17—H17B	109.5
C6—C7—S2	118.97 (15)	H17A—C17—H17B	109.5
C8—C7—S2	120.84 (14)	C16—C17—H17C	109.5
O6—C8—C9	125.04 (18)	H17A—C17—H17C	109.5

O6—C8—C7	114.81 (17)	H17B—C17—H17C	109.5
C9—C8—C7	120.14 (18)	C16—C18—H18A	109.5
C8—C9—C10	120.50 (19)	C16—C18—H18B	109.5
C8—C9—H9A	119.8	H18A—C18—H18B	109.5
C10—C9—H9A	119.8	C16—C18—H18C	109.5
C9—C10—C1	121.66 (19)	H18A—C18—H18C	109.5
C9—C10—C5	119.23 (18)	H18B—C18—H18C	109.5
O3—S1—N1—C12	−45.7 (2)	C5—C6—C7—S2	−178.34 (15)
O2—S1—N1—C12	−175.98 (18)	O4—S2—C7—C6	−3.88 (19)
C3—S1—N1—C12	69.3 (2)	O5—S2—C7—C6	−132.83 (16)
O4—S2—N2—C16	53.43 (18)	N2—S2—C7—C6	112.02 (16)
O5—S2—N2—C16	−177.42 (15)	O4—S2—C7—C8	178.22 (16)
C7—S2—N2—C16	−60.57 (18)	O5—S2—C7—C8	49.27 (18)
C11—O1—C2—C1	3.5 (4)	N2—S2—C7—C8	−65.88 (18)
C11—O1—C2—C3	−175.7 (2)	C15—O6—C8—C9	−3.8 (3)
C10—C1—C2—O1	179.1 (2)	C15—O6—C8—C7	176.08 (18)
C10—C1—C2—C3	−1.7 (3)	C6—C7—C8—O6	−177.07 (18)
O1—C2—C3—C4	−177.49 (19)	S2—C7—C8—O6	0.8 (2)
C1—C2—C3—C4	3.2 (3)	C6—C7—C8—C9	2.8 (3)
O1—C2—C3—S1	0.4 (3)	S2—C7—C8—C9	−179.31 (16)
C1—C2—C3—S1	−178.88 (18)	O6—C8—C9—C10	177.37 (19)
O3—S1—C3—C4	−14.70 (19)	C7—C8—C9—C10	−2.5 (3)
O2—S1—C3—C4	114.23 (17)	C8—C9—C10—C1	−179.6 (2)
N1—S1—C3—C4	−131.72 (16)	C8—C9—C10—C5	−0.1 (3)
O3—S1—C3—C2	167.35 (17)	C2—C1—C10—C9	177.6 (2)
O2—S1—C3—C2	−63.72 (19)	C2—C1—C10—C5	−1.8 (3)
N1—S1—C3—C2	50.3 (2)	C6—C5—C10—C9	2.5 (3)
C2—C3—C4—C5	−1.2 (3)	C4—C5—C10—C9	−175.71 (19)
S1—C3—C4—C5	−179.20 (15)	C6—C5—C10—C1	−178.05 (19)
C3—C4—C5—C6	179.59 (19)	C4—C5—C10—C1	3.7 (3)
C3—C4—C5—C10	−2.2 (3)	S1—N1—C12—C13	−100.2 (2)
C4—C5—C6—C7	175.95 (18)	S1—N1—C12—C14	137.2 (2)
C10—C5—C6—C7	−2.2 (3)	S2—N2—C16—C17	−111.90 (18)
C5—C6—C7—C8	−0.4 (3)	S2—N2—C16—C18	123.47 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.88	2.00	2.821 (2)	154
N2—H2*B*···O5^{ii}	0.88	2.22	3.001 (2)	148
N2—H2*B*···O6^{ii}	0.88	2.53	3.235 (2)	138

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*, −*y*+2, −*z*+1.